Abstract Submitted for the PSF09 Meeting of The American Physical Society

Role of surface band structures in the survival of anions scattered off plane and nano-stepped surfaces ANDREW SCHMITZ, JOHN SHAW, HI-MADRI CHAKRABORTY, Northwest Missouri State University, Maryville, MO 64468, UWE THUMM, Kansas State University, Manhattan, KS 66502 — Resonant charge transfer between ions and metal surfaces is a valuable tool to explore the surface electronic structure. Using the Crank-Nicholson propagation [1] we solve the time-dependent Schroedinger equation to simulate the dynamic electron redistribution during the scattering of a hydrogen anion from plane and nano-stepped vicinal metal surfaces. The electronic evolution during the scattering and the final ion survival probability as a function of the projectile's incident angle are calculated. We find that the survival of the ion reflected from a plane surface is very sensitive to the component of the projectile speed perpendicular to the surface. For a host of simple metal surfaces, unique roles of the band gap and the image states are uncovered that enable a nearly universal energy-scaling of the ion-survival. For the stepped surfaces, conversely, the survival is found to depend critically on the ion speed parallel to the surface, resulting in rich structures in the survival probability.

[1] Chakraborty et al., *Phys. Rev.* A **70**, 052903 (2004).

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